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LANDAU SPECTRUM AND LINE BROADENING IN REAL METALS

by

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ABSTRACT

The energy spectrum and level broadening of conduction electrons in the presence of a uniform magnetic field has been studied within the framework of the effective Hamiltonian formalism. A simple model which demonstrates the important ideas involved has been chosen. WKB solutions to the effective Hamiltonian have been found for this model. By using connection formulas which are accurate for all energies, we have shown how the degeneracies among the WKB solutions in different zones in reciprocal space are removed. These connection formulas were expressed in terms of a transmission amplitude p and a reflection amplitude q.

It has been found that the Landau levels are given accurately by the Onsager rules and are essentially discrete except in the immediate vicinity of open orbits. The transition between the nearly discrete closed orbit region and the continuous open orbit region was found to occur in an energy range of only a few $\hbar\omega_c$.

The eigenvalues and eigenfunctions of the effective Hamiltonian were shown to be consistent with the requirements of a group theoretical treatment of the exact Hamiltonian. Therefore, it has been concluded that no source of level broadening in a perfect crystal (other than interband effects) has been omitted.

A justification of Pippard's linear network model for magnetic breakdown has been given within the effective Hamiltonian formalism. The effects of internal strains and dislocations on the energy levels have also been considered.

I. INTRODUCTION

One of the most fruitful methods of determining the electronic properties of metals has been the study of their response to a magnetic field. In particular, the de Haas-van Alphen effect has given detailed information about the Fermi surfaces of many of the common metals. The interpretation of these and other related effects has been based upon unusually simple arguments. For example, the rules of Onsager (1952) which quantize the allowed areas in $\underline{k}$-space of the electron orbits and the equivalent Bohr-Sommerfeld rules employed by Lifshitz and Kosevich (1956) have been quite successful in explaining the de Haas-van Alphen effect.

In essence, we suppose that $\underline{r}$ and $\underline{p} = \hbar\underline{k} - \frac{e}{c}\underline{A}$ are canonically conjugate variables and the dispersion law or energy function for a band, $E(\underline{k})$, serves as the Hamiltonian in a semiclassical treatment (Wannier 1962). To introduce quantum mechanics into the problem, we can either use the Bohr-Sommerfeld rules (Onsager 1952) or the Correspondence Principle where $\underline{p}$ is replaced by $-i\hbar\nabla$ (Lifshitz and Kaganov 1960). The latter approach is called the effective Hamiltonian formalism (Wannier 1962). The equivalent of the Schrödinger equation is then

$$E\left(-i\nabla + \frac{e}{\hbar c}\underline{A}\right)\Psi(\underline{r}) = E\Psi(\underline{r}) \ . \qquad (1.1)$$

The validity of the semiclassical treatment or the effective Hamiltonian formalism can not be seriously doubted in most instances because of the overwhelming wealth of experimental information which has been so successfully interpreted by their use. The formal or theoretical justification is, however, only mildly convincing.

In 1930, the classic work of Landau appeared in which he solved the problem of the free electron in a magnetic field. Shortly thereafter, Peierls (1933) carried out the first analysis of a Bloch electron in a magnetic field. He found that, within the framework of the tightbinding approximation, (1.1) gave the correct energy levels.

Luttinger considered the problem again in 1951 in terms of Wannier functions, and justified (1.1) only when interband matrix elements could be neglected. Adams (1952) showed that interband matrix elements had to be considered and found (Adams 1953) that, for bands which are separated by only a small energy gap, interband effects could be an important contribution to the steady diamagnetism.

Luttinger and Kohn (1955) found that for states near the bottom (or the top) of a band, an effective mass approximation to (1.1) was useful in describing impurity states in a semiconductor. Kohn (1959), in a complicated extension of this work, gave the first of the more recent attempts to justify a form of (1.1). He found that by making a series of unitary transformations he could eliminate interband matrix elements to any order of H and thereby retain the form (1.1). In Kohn's treatment, the operator in (1.1) is replaced by a power series in H:

$$\epsilon_0(\underline{P}) + \frac{H}{c}\epsilon_1(\underline{P}) + \frac{H^2}{c^2}\epsilon_2(\underline{P}) + \ldots \qquad (1.2)$$

where $\underline{P} = i\nabla + \frac{e}{\hbar c}\underline{A}$. The lowest order term, $\epsilon_0(\underline{P})$, is just the energy band function $E(\underline{P})$. The question of the convergence of this procedure to eliminate interband matrix elements was not answered.

Blount (1962) reexamined the problem and purported to have simplified Kohn's original work. Blount established the asymptotic convergence of

Kohn's treatment and considered more general band structures. Roth (1962), in a similar paper, also tried to simplify Kohn's work. Wannier (1960, 1962) looked at the problem for both electric and magnetic fields.

The major difficulty in the effective Hamiltonian formalism is now and was throughout the past 30 years the question of the importance of the interband matrix elements. The first experimental evidence of the importance of interband effects was pointed out by Cohen and Falicov in 1961. They suggested that the giant orbits observed in the de Haas-van Alphen effect in Mg were due to orbits composed of pieces of the Fermi surface in two different bands. The process of tunneling from one band to another was called magnetic breakdown. Since then, Pippard (1962, 1964, 1965) and Chambers (1966) have treated the energy levels and Falicov and Stachowiak (1966) have treated the amplitudes of de Haas-van Alphen oscillations of a system of orbits coupled by magnetic breakdown.

In the absence of serious interband effects such as breakdown, one can ask what are the energy levels given by (1.1). The first solution to (1.1) for a case other than parabolic bands was obtained by Harper in 1955. He considered a simple cubic crystal with a tightbinding band structure:

$$E(\underline{k}) = E_o \, (\cos ak_x + \cos ak_y + \cos ak_z) \quad . \tag{1.3}$$

Harper solved the equivalent Schrödinger equation by a finite difference technique. Brailsford (1957), subsequently, repeated the calculation for a generalization of (1.3) and found Harper's results in error. Brailsford found that the energy levels were given quite accurately by the Onsager rules and were essentially discrete except for energies near open orbits. Chambers (1956) showed that the conclusions of Brailsford were correct for

band shapes other than tightbinding bands, although no detailed treatment of the energy levels was given.

Zil'berman (1957a, 1957b, 1958) proceeded independently of the work described above. He derived an effective Hamiltonian formalism of his own and examined the energy spectrum. The level broadening obtained by Zil'berman depended rather strongly upon the approximations that he made, but in general, the level widths were found to be quite small in the discrete region of closed orbits.

Azbel' (1964), also independently of most of the work described above, found a very complicated substructure of the Landau levels. His work is, as he pointed out, not experimentally significant because crystal imperfections, impurities, and other scattering processes will obscure any such substructure. There is, however, the essence of the answer to the energy level problem buried in his work, although he did not consider it in any detail.

A completely different approach has been tried by Brown (1964) and by Zak (1964a, 1964b, 1964c, 1965). They have studied the exact Schrödinger equation

$$\frac{\hbar^2}{2m}\left(-i\nabla + \frac{e}{\hbar c}\underline{A}\right)^2 X(\underline{r}) + V(\underline{r})\, X(\underline{r}) = EX(\underline{r}) \quad , \tag{1.4}$$

where $V(\underline{r})$ is the lattice potential. Brown found the irreducible representations of the exact Hamiltonian and Zak treated the lattice potential as a perturbation using the proper symmetry-adapted wave functions. The perturbation approach can only establish the existence of broadening at best. The whole approach fails for even the most free-electron-like metals because the matrix elements of the lattice potential are much larger than

$\hbar\omega_c$, the separation of the unperturbed levels. Likewise, group theory can not establish more than the general nature of the solution.

It seems reasonable to conclude that the position of the energy levels is quite well established in most circumstances by the Onsager rules. The question of the broadening is, as Kohn (1959) pointed out, not clearly answered. There are, of course, many contributions to the level broadening in a real crystal in addition to the natural line width that would be found in a perfect crystal. The effects of impurities has been treated by Dingle (1952a, 1952b) and is known as Dingle broadening. The effects of crystal imperfections has been treated only in brief by Pippard (1965) and Chambers (ca. 1967) and may be important.

The purpose of this work is to examine in detail the energy spectrum and the solutions to (1.1) in the absence of any scattering mechanisms. The general philosophy will be that the effective Hamiltonian formalism is valid within the limitations discussed above, and the validity of any conclusions reached will be subject to the validity of (1.1).

II. EFFECTIVE HAMILTONIAN FORMALISM

Let us consider a nondegenerate band, for which the energy is given by $E(\underline{k})$ in the absence of any external fields. A band is nondegenerate if, at any $\underline{k}$, no other band has the same energy $E(\underline{k})$. It may be that the energy range of the band will overlap the energy range of an adjacent band, but, so long as the bands do not touch at any point in $\underline{k}$-space, they are nondegenerate.

The energy band function $E(\underline{k})$, in the repeated zone scheme (Ziman 1964, p. 78-79), is periodic in reciprocal space. If $\underline{K}$ is a reciprocal lattice vector, then

$$E(\underline{k} + \underline{K}) = E(\underline{k}) \quad . \tag{2.1}$$

Another way to express (2.1) is to write

$$E(\underline{k}) = \sum_j W(\underline{R}_j)\, e^{i\underline{k} \cdot \underline{R}_j} \quad , \tag{2.2}$$

where the sum is over all lattice vectors of the direct lattice, $\underline{R}_j$. The coefficients $W(\underline{R}_j)$ determine the band structure.

The effective Hamiltonian in the absence of any external fields is obtained by replacing $\underline{k}$ by $-i\nabla$ in (2.2). The operator $e^{i\underline{R}_j \cdot (-i\nabla)}$ is simply a translation operator $T(\underline{R}_j)$,

$$T(\underline{R}_j)\, \Psi(\underline{r}) = \Psi(\underline{r} + \underline{R}_j) \tag{2.3}$$

The equivalent of the Schrödinger equation is

$$\begin{aligned} E(-i\nabla)\, \Psi\, (\underline{r}) &= \sum_j W(\underline{R}_j)\, T(\underline{R}_j)\, \Psi(\underline{r}) \quad , \\ &= E\, \Psi(\underline{r}) \quad . \end{aligned} \tag{2.4}$$

(When E is written without any argument, it stands for an eigenvalue.) It is easy to show that the eigenfunctions of (2.4) are plane waves and the eigenvalues are given by $E(\underline{k})$.

It should be noted that $\Psi(\underline{r})$ is not the actual wave function which would be a solution to the exact Schrödinger equation (1.4). $\Psi(\underline{r})$ is the wave function only in a certain representation, that of the effective Hamiltonian. As an example of the relationship between $\Psi(\underline{r})$ and the actual wave function, say $X(\underline{r})$, in the tightbinding approximation (Ziman 1964, p. 80-85), we have

$$X(\underline{r}) = \sum_j \Psi(\underline{R}_j)\, u(\underline{r} - \underline{R}_j) \quad , \tag{2.5}$$

where $u(\underline{r})$ is an atomic orbital.

When an external electric field exists, the effective Hamiltonian becomes $E(-i\nabla) + V(\underline{r})$, where $-\nabla V(\underline{r})$ is the electric field. This form has been useful for impurity states in semiconductors (Luttinger and Kohn 1955).

In the presence of a magnetic field $\underline{H}$, the effective Hamiltonian is $E(-i\nabla + \frac{e}{\hbar c}\underline{A})$, where we take the vector potential to be

$$\underline{A} = \frac{1}{2}\,\underline{H} \times \underline{r} \quad . \tag{2.6}$$

The gauge (2.6) is convenient because the translation operators $T(\underline{R}_j)$ commute with $\underline{A}$ (Brown 1964), and the effective Hamiltonian operator is unambiguously defined. The eigenvalue equation is then

$$\begin{aligned} E(-i\nabla + \tfrac{e}{\hbar c}\underline{A})\,\Psi(\underline{r}) &= \sum_j W(\underline{R}_j)\, \exp \tfrac{i}{2}\underline{R}_j \cdot (\underline{b}\times\underline{r})\, T(\underline{R}_j)\,\Psi(\underline{r}) \quad , \\ &= E\,\Psi(\underline{r}) \quad , \end{aligned} \tag{2.7}$$

where $\underline{b} = \frac{e\underline{H}}{\hbar c}$. ($\underline{b}$ is parallel to $\underline{H}$ since we have taken e as positive.)

The differential equation (2.7) is similar to the differential equation for a free electron in a magnetic field,

$$\frac{\hbar^2}{2m} (-i\nabla + \frac{e}{\hbar c} \underline{A})^2 X(\underline{r}) = EX(\underline{r}) \quad , \tag{2.8}$$

in that the differential operator on the left-hand side of both (2.7) and (2.8) is a function only of $-i\nabla + \frac{e}{\hbar c} \underline{A}$. Following Zak (1965) who gave a solution to (2.8) (because of the large degeneracy in the solutions to (2.8), many forms are possible), we write $\Psi(\underline{r})$ in such a form as to reduce (2.7) to an equation in one variable,

$$\Psi(\underline{r}) = e^{ik_z z + ik_x x - i\frac{b}{2} xy} \phi(y - \frac{k_x}{b}) \quad . \tag{2.9}$$

We choose the z-axis to be along $\underline{H}$. It is convenient to pick the y-axis to be along the shortest reciprocal lattice vector, say $\underline{K}_1$, in the xy plane (the plane perpendicular to $\underline{H}$). Since the motion of an electron along the magnetic field is unaffected by the field, k_z is a good quantum number. From group theory (Zak 1965), we know that we can also pick k_x (or k_y, but not both) as a good quantum number. The factor $e^{-i\frac{b}{2}xy}$, in effect, transforms the gauge from that of (2.6) to

$$\underline{A} = (-Hy, 0, 0) \quad . \tag{2.10}$$

Substituting (2.9) into (2.7) and shifting the origin of y to $\frac{k_x}{b}$, we can show that $\phi(y)$ satisfies the one dimensional equation

$$\sum_j W(\underline{R}_j) \exp i(k_z Z_j - \frac{b}{2} X_j Y_j - byX_j) T(Y_j) \phi(y) = E\phi(y) \quad , \tag{2.11}$$

where $\underline{R}_j = (X_j, Y_j, Z_j)$ and

$$T(Y_j)\ \phi(y) = \phi(y + Y_j) \quad . \tag{2.12}$$

As in the free electron case, the eigenvalue is independent of k_x.

One might be tempted at this point to try to recover the free electron case by specializing to parabolic bands. We can not do this immediately, however, for the simple reason that the expansion (2.2) is periodic in reciprocal space and involves (for parabolic bands) a number of degeneracies at the Brillouin zone boundary. For example, at the point $\frac{1}{2}\underline{K}_1$, in a simple cubic crystal, the single band approximation we have assumed no longer is valid because the bands touch. (See Figure 1.) If we include interband effects, as in Pippard's analysis of magnetic breakdown (1962), then we can recover the free electron problem and obtain the correct eigenvalues,

$$\frac{\hbar^2 k_z^2}{2m} + (n + 1/2)\ \hbar\omega_c \text{ , where } \omega_c = \frac{eH}{mc} \quad .$$

In simple semiconductors where the conduction band is parabolic near $\underline{k} = 0$, it is well-known that an effective mass approximation to (2.7) is useful (Luttinger and Kohn 1955). It is instructive to show how to obtain the effective mass equation starting from (2.7) in view of the previous paragraph. The essential difference between the semiconductor problem and the free electron problem is that we are interested in only a restricted region near the bottom of the band in the semiconductor case.

We think of constructing $\Psi(\underline{r})$ by superimposing a number of plane waves as in a Fourier transform,

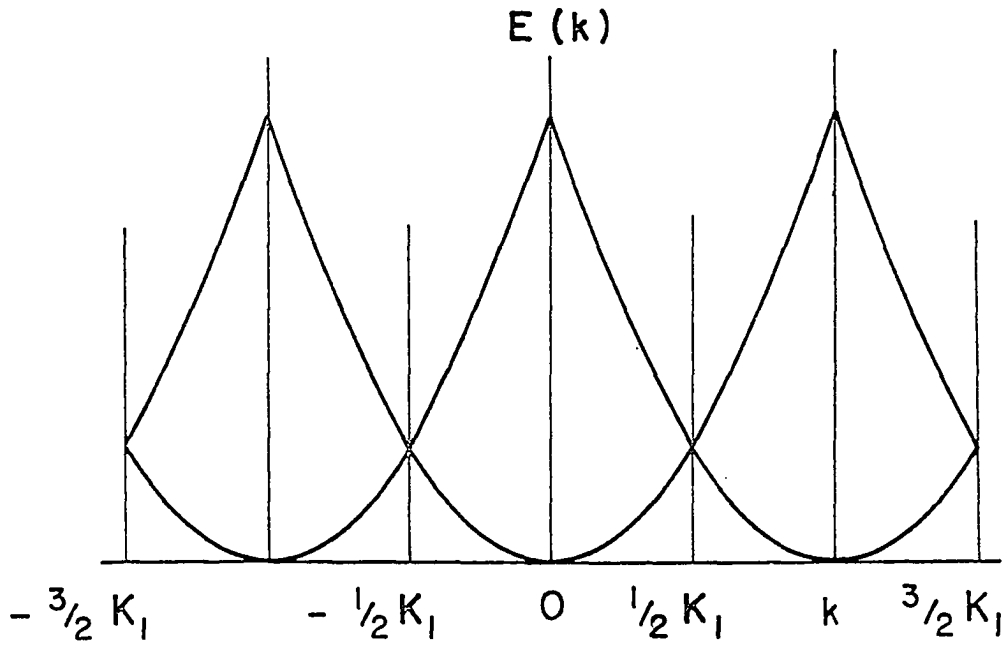


Figure 1. Free electron energy bands in the repeated zone scheme.

$$\Psi(\underline{r}) = \int d^3k \, e^{i\underline{k} \cdot \underline{r}} \, \Phi(\underline{k}) \quad . \tag{2.13}$$

So long as $\Phi(\underline{k})$ is large for only small values of $\underline{k}$ (as for states near the bottom of the band), it is proper to expand $E(\underline{k})$ about $\underline{k} = 0$ first and then replace $\underline{k}$ by $-i\nabla + \frac{e}{\hbar c}\underline{A}$. In such a manner, it is easy to obtain the effective mass equation

$$\frac{\hbar^2}{2m^*}\left(-i\nabla + \frac{e}{\hbar c}\underline{A}\right)^2 \Psi(\underline{r}) = E\Psi(\underline{r}) \quad , \tag{2.14}$$

where for small $\underline{k}$

$$E(\underline{k}) = \frac{\hbar^2 k^2}{2m^*} \quad . \tag{2.15}$$

In other words, when the energy is small relative to the bottom of the band, a form such as (2.14) is correct.

Finally, it should be noted that the solutions to (2.11) must be of the Bloch form (in one dimension) because the differential operator on the left-hand side is periodic in y with period $r_1 = \frac{K_1}{b}$. As a consequence, we can label $\phi(y)$ with a continuous index Q, where the significance of Q is given by

$$\phi_Q(y + r_1) = e^{iQr_1} \phi_Q(y) \quad . \tag{2.16}$$

The range of Q is restricted to $\frac{2\pi}{r_1}$.

In general, $\phi(y)$ will be labeled with a discrete index n, as in the free electron case, and the continuous index or wavenumber Q. Each n corresponds to a particular Landau level. The dependence of the energy on Q corresponds to the broadening or the natural width of the levels.

III. ONE-DIMENSIONAL COUPLING IN A SIMPLE MODEL

The solution to the one-dimensional equation (2.11) for an arbitrary magnetic field direction in an arbitrary band structure would be a difficult problem. Fortunately, we can make a number of simplifying assumptions to obtain a model which demonstrates the important ideas involved. In view of the absence of experimental data concerning the details of the Landau spectrum (energy spectrum) and level broadening, it does not seem worthwhile at this point to worry about complicated Fermi surface topology, but rather to emphasize only certain basic features.

For our model, we assume that the band structure is such that

$$E(\underline{k}) = E_1(k_x) + E_2(k_y) + E_3(k_z) \quad , \tag{3.1}$$

where $\underline{H}$ is directed along the z-axis. $E_1(k_x)$ and $E_2(k_y)$ are, of course, periodic (with periods K_1 and K_2 respectively) and we take them to be even about the origin ($E(-k) = E(k)$). Furthermore, we assume that $E_1(k_x)$ and $E_2(k_y)$ are simple functions with maxima at the zone boundaries ($\pm \frac{1}{2} K_1$ and $\pm \frac{1}{2} K_2$). $E_3(k_z)$ can be considered a constant of the motion since k_z is a constant of the motion. For convenience, we absorb $E_3(k_z)$ into the eigenvalue E.

Separating the k_x and k_y variables in (3.1) eliminates the cross terms $e^{-i\frac{b}{2} X_j Y_j}$ in (2.11) because $W(\underline{R}_j)$ vanishes unless X_j or $Y_j = 0$. In the general problem, the cross terms must be considered, but they cause no real difficulty. The effective Hamiltonian then becomes the sum of two terms, which can be looked upon as a kinetic energy term in operator form,

$$E_2(-i\frac{d}{dy}) = \sum_j W(Y_j)\, T(Y_j) \quad , \tag{3.2}$$

and a potential energy term,

$$V_1(y) = E_1(by) \quad . \tag{3.3}$$

$V_1(y)$ is periodic with period $r_1 = \frac{K_1}{b}$ and varies between 0 and W_1 (see Figure 2). The kinetic energy function $E_2(k_y)$ is similar and varies between 0 and W_2. We suppose that W_2 is sufficiently larger than W_1, so that a sizeable region of open orbits exists (T_3, T_4 and T_5 in Figure 3).

The equivalent Schrödinger equation (2.11) is for our model

$$E_2(-i\frac{d}{dy})\,\phi(y) + V_1(y)\,\phi(y) = E\,\phi(y) \quad . \tag{3.4}$$

The period of the function $V_1(y)$, r_1, is quite large on an atomic scale (typically 10^2 to 10^3 lattice constants), and $V_1(y)$ is, therefore, a slowly varying function. Normally, we will be concerned with energies in the vicinity of the Fermi energy, so it is certainly proper to regard (3.4) as being in the quasi-classical region. Hence, a WKB approach is indicated (Landau and Lifshitz 1958, p. 157-185, Schiff 1955, p. 184-193). The WKB approximation has been used by several authors (e.g. Zil'berman 1957b, 1958, Blount 1962), but in a slightly different way.

One might object that the kinetic energy operator in (3.2) and the equation (3.4) are not in the standard WKB form, but it is an easy manner to show that the WKB wave function,

$$\phi(y) = \frac{1}{\sqrt{v}} \exp\left(\pm i \int^y k(y')\, dy'\right) \quad , \tag{3.5}$$

is an approximate solution to (3.4) if we take k(y) to be given implicitly

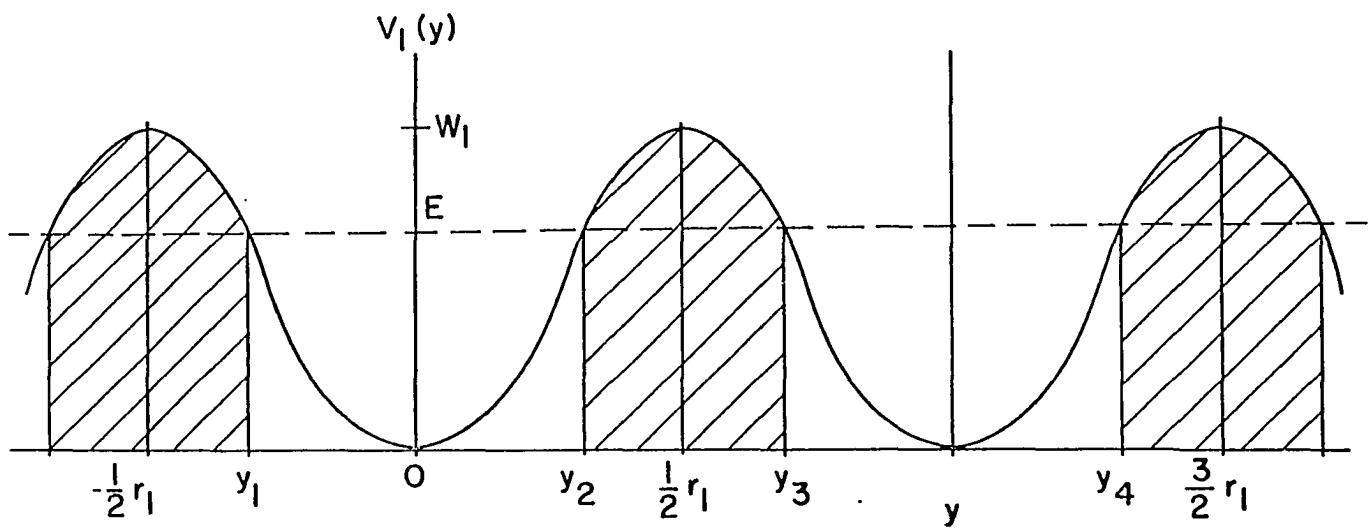


Figure 2. Potential energy function for a simplified model of the effective Hamiltonian formalism ($V_1(y) = E_1(by)$). Shaded portion indicates the region where the wave function is exponentially increasing or decreasing.

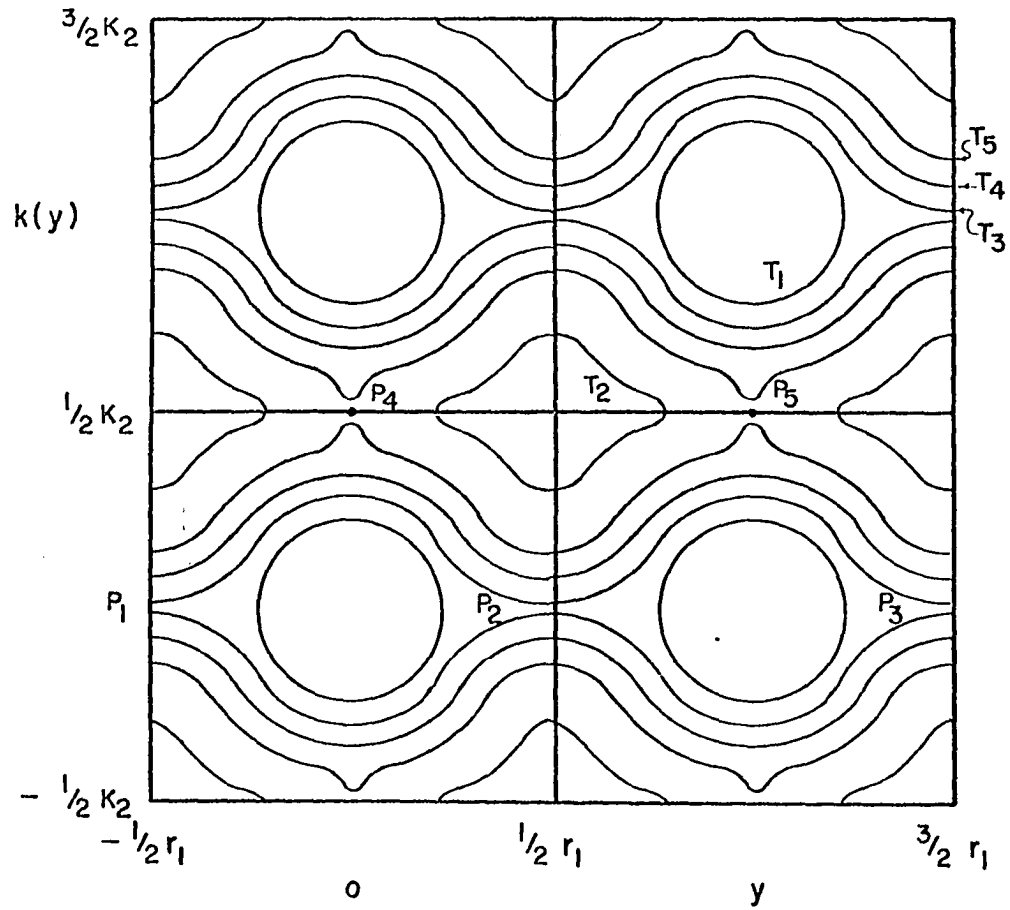


Figure 3. Contours of constant energy in the k(y)-y plane ($E_1(by)) + E_2(k(y)) = E$). T_1: closed electron orbit; T_2: closed hole orbit; T_3, T_4 and T_5: open orbits. P_1, P_2, P_3, P_4 and P_5: points where orbits can couple.

by

$$E_1(k(y)) + V_1(y) = E \quad , \tag{3.6}$$

and

$$v = \frac{1}{\hbar} \left| E_1'(k(y)) \right| \quad . \tag{3.7}$$

(The prime denotes differentiation with respect to the argument.) Contours of constant energy in the k(y) - y plane which define k(y) are shown in Figure 3.

For energies less than W_1, the wave function is oscillatory in the valleys between the turning points where $V_1(y) < E$ and exponentially increasing or decreasing in the region where $V_1(y) > E$ (see Figure 3). The procedure in the ordinary WKB approximation would then be to connect the solutions in the adjacent valleys via the connection formulas and to determine the eigenvalues E by imposing the Bloch condition (2.16). Such a calculation was carried out, and it was found that the energy levels were given by the usual semiclassical quantization scheme (Ziman 1964, p. 273).

$$\int_{y_1}^{y_2} k(y)\, dy = (n + \tfrac{1}{2})\, \pi \quad , \tag{3.8}$$

and the dependence of the energy levels on Q (the broadening of the levels) was proportional to the probability to tunnel through the barrier, $\exp\left(-\int_{y_2}^{y_3} |k(y)|dy\right)$. Hence, the broadening was found to be extremely small except for E near W_1, and this result is in general agreement with the work of other authors which has been discussed in the introduction.

When the probability to tunnel through the barrier is negligible, each

eigenstate can be thought of as being localized in some valley. When the coupling between the states in adjacent valleys is negligible, all states are degenerate, and the levels are discrete. When the tunneling probability or coupling is not negligible, the degeneracies are removed and the discrete levels are broadened. Such is the case whether the coupling is intraband coupling, as discussed above, or interband coupling as in magnetic breakdown.

Since the WKB connection formulas and transmission coefficient (tunneling probability) are not accurate for energies near the top of the barrier or above the barrier, it was desirable to have a better approximation in this region where all the interesting effects take place. Away from the turning points, the WKB solutions are certainly accurate enough for our purposes. It is in the neighborhood of the turning points where a more careful analysis is necessary in order to obtain the proper connection between the solutions in adjacent valleys.

Azbel' (1964) gave a cursory treatment of the problem, but did not develop it enough to be of any help in the present investigation. The same type of barrier problem for the simpler kinetic energy operator $-\frac{\hbar^2}{2m}\frac{d^2}{dy^2}$ has been solved by Miller and Good (1953). The additional complications introduced by the operator $E_2(-i\frac{d}{dy})$ are, however, minor, and the analysis of Miller and Good will be useful.

For y near $\frac{1}{2} r_1$, we can expand the potential about its local maximum:

$$V_1(y) = W_1 - \frac{\hbar^2 b^2}{2m_1} (y - \tfrac{1}{2} r_1)^2 + \ldots \quad . \tag{3.9}$$

Since the kinetic energy, $E_2(k(y))$, is small for y near $\frac{1}{2} r_1$ (most of the

energy is potential energy), it is permissible to write

$$E_2\,(k(y)) = \frac{\hbar^2 k^2(y)}{2m_2^*} + \ldots \quad . \tag{3.10}$$

The effective mass m_1 is defined as positive, since the appropriate minus sign appears in (3.9), and the asterisk on m_2^* designates an effective mass at the bottom of the band.

In a restricted region around $\frac{1}{2} r_1$, then

$$\frac{\hbar^2 k^2(y)}{2m_2^*} + W_1 - \frac{\hbar^2 b^2}{2m_1} (y - \tfrac{1}{2} r_1)^2 = E \quad . \tag{3.11}$$

If we replace $k(y)$ by $-i\frac{d}{dy}$ in (3.11) and operate on $\phi(y)$, we obtain an equation which is correct for y near $\frac{1}{2} r_1$, and which can be solved exactly,

$$-\frac{\hbar^2}{2m_2^*} \frac{d^2\phi}{dy^2} - \frac{\hbar^2 b^2}{2m_1} (y - \tfrac{1}{2} r_1)^2 \phi = (E - W_1)\phi \quad . \tag{3.12}$$

If we let $$S = \left(\frac{m_2^*}{m_1} b^2\right)^{1/4} (y - \tfrac{1}{2} r_1)$$

and $$a = 2 \frac{(m_1 m_2^*)^{1/2}}{m} \left(\frac{E - W_1}{\hbar\omega_c}\right) ,$$

where $\omega_c = \frac{eH}{mc}$, and m is the free electron mass, then (3.12) becomes

$$\frac{d^2\phi}{dS^2} + (a + S^2)\,\phi = 0 \quad . \tag{3.13}$$

The equation (3.13) arises when the scalar Helmholtz equation is separated in parabolic coordinates (Morse and Feshbach 1953, p. 1398-1405).

For every value of a, there are two solutions (Miller and Good 1953)

$$\phi_1 = D_{1/2(ia-1)}\left(\sqrt{2}\, S\, e^{-i\pi/4}\right) \quad , \tag{3.14}$$

and

$$\phi_2 = D_{1/2(-ia-1)}\left(\sqrt{2}\, S\, e^{i\pi/4}\right) \quad . \tag{3.15}$$

The functions $D_n(z)$ are defined by Whittaker and Watson (1947, p. 347), but only their asymptotic form will concern us.

The general WKB solution will be a linear combination of the solutions (3.7). For $y > y_3$, we write

$$\phi(y) = \frac{B_1}{\sqrt{V}} \exp\left(i \int_{y_3}^{y} k\,dy\right) + \frac{B_2}{\sqrt{V}} \exp\left(-i \int_{y_3}^{y} k\,dy\right) \quad , \tag{3.16}$$

and for $y < y_2$,

$$\phi(y) = \frac{A_1}{\sqrt{V}} \exp\left(i \int_{y}^{y_2} k\,dy\right) + \frac{A_2}{\sqrt{V}} \exp\left(-i \int_{y}^{y_2} k\,dy\right) \quad . \tag{3.17}$$

(For convenience, the argument y in k(y) and the primes on the variable of integration have been dropped.)

In the region where the solutions (3.14) and (3.15) join onto the WKB solutions (3.16) and (3.17), it is reasonable to use the asymptotic form of ϕ_1 and ϕ_2 . From Miller and Good (1953), we have for S large and positive (with an appropriate normalization),

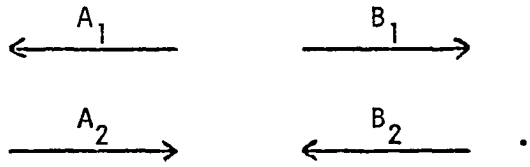
$$\phi_1 \rightarrow \frac{e^{1/2\ a\pi}}{\sqrt{V}} \exp\left(i \int_{y_3}^{y} k\,dy\right) \quad , \tag{3.18}$$

and for S large and negative,

$$\phi_1 \rightarrow \frac{C\, e^{1/4\, a\pi}}{\sqrt{V}} \exp\left(-i \int_y^{y_2} k\,dy\right) - \frac{i}{\sqrt{V}} \exp\left(i \int_y^{y_2} k\,dy\right) , \qquad (3.19)$$

where $$C = \left(\frac{2}{\pi}\right)^{1/2} \left(\frac{|a|}{2e}\right)^{-1/2ia} \Gamma\left(\frac{1}{2} + \frac{1}{2} ia\right) \cosh \frac{1}{2} a\pi \ . \qquad (3.20)$$

The second solution, ϕ_2 , gives the complex conjugate of (3.18) and of (3.19). The solution (3.18) corresponds to a wave traveling to the right, away from the barrier in the region $y > y_3$ (since the phase is increasing as y increases), whereas (3.19) is the sum of two terms, the first being a wave traveling to the right, toward the barrier in the region $y < y_2$, and the second being a wave traveling to the left and away from the barrier $(y < y_2)$. Symbolically, we have



Let us now use the notation that Pippard (1962) used in the analogous situation in magnetic breakdown. First, assume that B_2 is zero so that we have only a transmitted wave for $y > y_3$. We write

$$B_1 = p\, A_2 \ , \qquad (3.21)$$

and

$$A_1 = q\, A_2 \ , \qquad (3.22)$$

where A_2 is the amplitude of the incoming wave for $y < y_2$, A_1 is the amplitude of the reflected wave, and B_1 is the amplitude of the transmitted wave. The factors p and q are the probability amplitudes (with definite phase) for

transmission and reflection. The transmission coefficient is $|p|^2$ and conservation of probability requires that $|p|^2 + |q|^2 = 1$. From (3.18) and (3.19), we have

$$p = C^{-1} e^{1/4\, a\pi} \quad , \tag{3.23}$$

and

$$q = -iC^{-1} e^{-1/4\, a\pi} \quad . \tag{3.24}$$

We can evaluate $|C|^2$ by imposing the conservation of probability,

$$|C|^2 = 2 \cosh \tfrac{1}{2} a\pi \quad . \tag{3.25}$$

From (3.23) and (3.25) we obtain the transmission coefficient

$$|p|^2 = \frac{1}{1+e^{-a\pi}} \quad . \tag{3.26}$$

In the limit of large, negative a, (3.26) agrees with the usual WKB tunneling probability.

If now we consider $A_2 = 0$, we can, with the help of (3.18) and (3.19) and the complex conjugates of (3.18) and (3.19), show that

$$A_1 = p\, B_2 \quad , \tag{3.27}$$

and

$$B_1 = q\, B_2 \quad . \tag{3.28}$$

(3.27) and (3.28) are to be expected since the barrier appears the same from either side.

Let us write $C = |C|\, e^{i\alpha}$, where from (3.20),

$$\alpha = \tfrac{1}{2} a \left(1 - \log \frac{|a|}{2}\right) + \arg \Gamma \left(\tfrac{1}{2} + \tfrac{1}{2} ia\right) \quad , \tag{3.29}$$

and from (3.25) ,

$$|C| = (2 \cosh \tfrac{1}{2} a\pi)^{1/2} \quad . \tag{3.30}$$

For $a = 0$, $\alpha = 0$, and from asymptotic expansion of $\Gamma(\frac{1}{2} + \frac{1}{2} ia)$ for large a (positive or negative)

$$\alpha = \frac{a}{4} \log \left(\frac{1 + a^2}{a^2}\right) - \frac{1}{6a} + \ldots \tag{3.31}$$

which goes to zero as $\frac{1}{12a}$ for large a.

We now write (3.23) and (3.24) as

$$p = e^{-i\alpha} (1 + e^{-a\pi})^{-1/2} \quad , \tag{3.32}$$

$$q = -i\, e^{-i\alpha} (1 + e^{a\pi})^{-1/2} \quad . \tag{3.33}$$

To connect the solutions in adjacent valleys, then, we merely employ p and q as in (3.21), (3.22), (3.27), and (3.28). We find

$$A_1 = q\, A_2 + p\, B_2 \quad ,$$

and

$$B_1 = p\, A_2 + q\, B_2 \quad . \tag{3.34}$$

Returning now to the calculation of the allowed energy levels, we rewrite (3.17) as

$$\phi(y) = \frac{A_2}{\sqrt{V}} \exp i\left(\int_{y_1}^{y} k dy - \xi\right) + \frac{A_1}{\sqrt{V}} \exp -i\left(\int_{y_1}^{y} k dy - \xi\right) , \tag{3.35}$$

where

$$\xi = \int_{y_1}^{y_2} k dy \quad . \tag{3.36}$$

When $a > 0$ $(E > W_1)$, we take $y_1 = -\frac{1}{2} r_1$ and $y_2 = \frac{1}{2} r_1$.

From the Bloch condition (2.16), we find

$$B_1 = A_2 \, e^{i(Qr_1 - \xi)} \quad ,$$

and

$$B_2 = A_1 \, e^{i(Qr_1 + \xi)} \quad . \tag{3.37}$$

Combining (3.34) and (3.37), we have

$$(1 - p \, e^{i(Qr_1 + \xi)}) \, A_1 - q \, A_2 = 0 \quad ,$$

and

$$q \, e^{i(Qr_1 + \xi)} \, A_1 + (p - e^{i(Qr_1 - \xi)}) \, A_2 = 0 \quad . \tag{3.38}$$

If 3.38) is to hold, the secular determinant must vanish. Whence, after some simple manipulations we find the quantization condition

$$\cos (\xi - \alpha) = \cos Qr_1 \, (1 + e^{-a\pi})^{-1/2} \quad . \tag{3.39}$$

For $Qr_1 = \frac{\pi}{2}$, (3.39) becomes the quantization condition for the centroid of the energy level,

$$\cos (\xi - \alpha) = 0$$

or

$$\xi = (n + \tfrac{1}{2}) \, \pi + \alpha \quad , \tag{3.40}$$

where n is an integer.

For $Qr_1 \neq \frac{\pi}{2}$, we set $\xi - \alpha = (n + \frac{1}{2})\pi + \Delta\pi$, to obtain

$$\sin \Delta\pi = (-1)^{n+1} \cos Qr_1 \, (1 + e^{-a\pi})^{-1/2} \quad . \tag{3.41}$$

When the coupling is negligible (a large and negative), Δ will be small

enough so that we can replace sin $\Delta\pi$ by $\Delta\pi$, and (3.41) becomes

$$\Delta\pi = (-1)^{n+1} \cos Qr_1 \, e^{-|a|\,\pi/2} \quad . \tag{3.42}$$

The range of Δ (denoted by δn), which gives the relative line width is, then, for weak broadening

$$\delta n = 2\, e^{-|a|\pi/2} \quad . \tag{3.43}$$

In general, the relative broadening is given by

$$\sin\left(\delta n \frac{\pi}{2}\right) = (1 + e^{-a\pi})^{-1/2} \quad . \tag{3.44}$$

For $a = 0$, $\delta n = \frac{1}{2}$; for a large and positive, δn becomes unity and the spectrum is continuous.

It is interesting to note that the function on the right-hand side of (3.44) is the square root of the Fermi-Dirac function (Ziman 1964, p. 118), which implies that the transition takes place over an energy range of only a few $\hbar\omega_c$, unless the effective mass $(m_1 m_2^*)^{1/2}$ is extremely small (see Figure 4).

The presence of the α term in (3.40), where α is given by (3.29), shifts the energy levels up slightly above W_1 ($a > 0$) and down slightly below W_1 ($a < 0$). For $|a|$ large, α is slowly varying and nearly vanishes. The only level which the α term will effect at all seriously is the level which falls closest to $a = 0$, where the derivative is singular.

At this point it is interesting to examine the line shapes of the energy levels. Several theoretical treatments of the influence of broadening on the de Haas-van Alphen effect have assumed the line shape to be

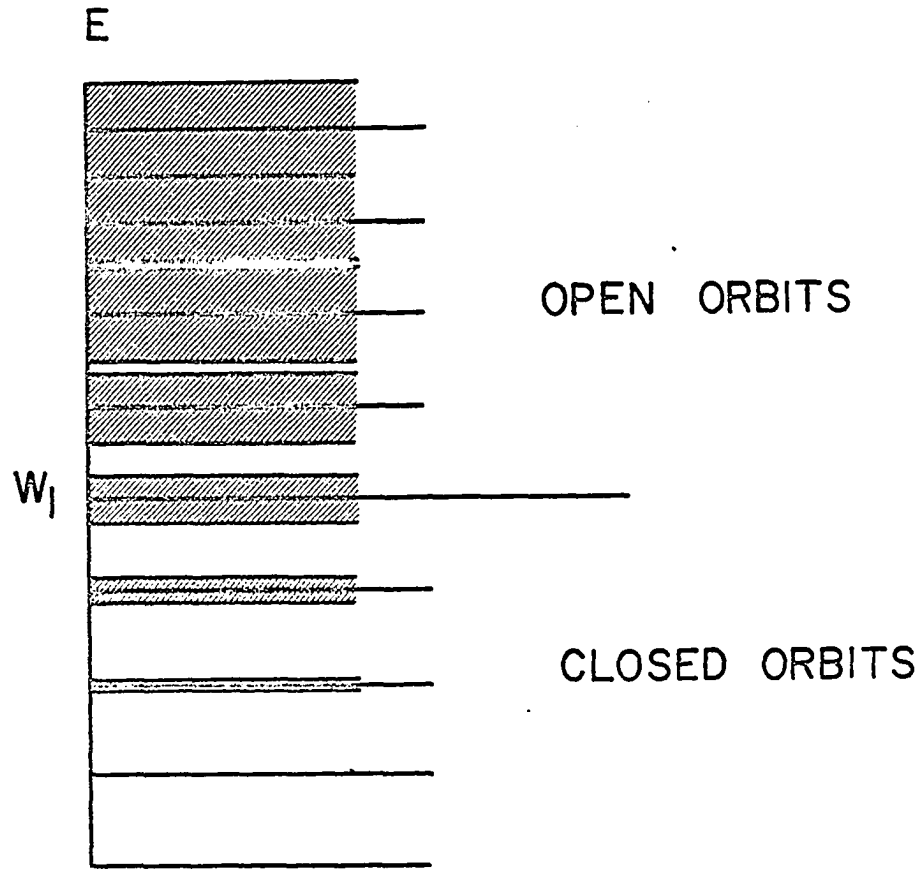


Figure 4. Landau level broadening in the transition region between open and closed orbits.

Lorentzian (Dingle 1952a, 1952b, Williamson, Foner and Smith 1964).

From (3.42) and (3.43), we have for weakly broadened lines

$$\Delta = \frac{1}{2}\,\delta n \cos Qr_1 \quad . \tag{3.45}$$

The density of states is proportional to $(\frac{d\Delta}{dQ})^{-1}$, so that we find the distribution function $f(\epsilon)$ describing the line shape to be given by (see Figure 5)

$$f(\epsilon) = (1 - \epsilon^2)^{-1/2} \quad , \qquad \epsilon^2 < 1 \quad ,$$

and $$f(\epsilon) = 0 \quad , \qquad \epsilon^2 > 1 \quad , \tag{3.46}$$

where ϵ is defined as

$$\epsilon = \frac{E - En}{\delta E} \quad . \tag{3.47}$$

E_n is the centroid of the nth level, and $2\delta E$ is the total width. At higher energies, where the broadening is pronounced, Δ approaches a linear function of Q. Consequently, the levels become rather broad and nearly uniform as we should expect for the continuous region of the energy spectrum.

So far we have considered only closed electron orbits and the open orbits which are close to them (T_1 and T_3 in Figure 3). When E exceeds W_2, open orbits no longer exist, and we have closed hole orbits (T_2). This means that the WKB solutions are not accurate near the origin when the energy is approximately W_2 or greater.

For y near y = 0 and k(y) near $\frac{1}{2} K_2$, $E_2(k(y))$ reaches a maximum, W_2, and we can expand

$$E_2(k(y)) = W_2 - \frac{\hbar^2}{2m_2}\,(k(y) - \tfrac{1}{2} K_2)^2 + \ldots \quad . \tag{3.48}$$

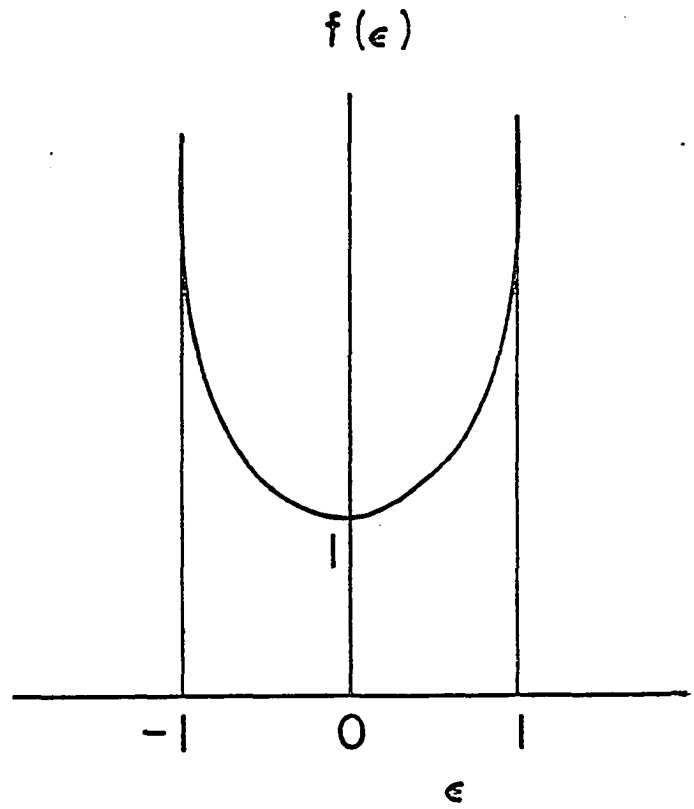


Figure 5. Shape of weakly broadened Landau levels. $f(\epsilon)$ is the distribution function or density of states function for a given energy level.

Likewise, the potential energy can be expanded for y small

$$V_1(y) = \frac{\hbar^2 b^2 y^2}{2m_1^*} + \ldots \quad . \tag{3.49}$$

Hence, we have, for y near the origin and k(y) near $\frac{1}{2} K_2$,

$$\frac{-\hbar^2}{2m_2} \left(k(y) - \tfrac{1}{2} K_2\right)^2 + W_2 + \frac{\hbar^2 b^2 y^2}{2m_1^*} = E \quad . \tag{3.50}$$

Replacing k(y) by $-i \frac{d}{dy}$ and operating on $\phi(y)$, we obtain after multiplication by -1,

$$\frac{-\hbar^2}{2m_2} \left(\frac{d}{dy} - \frac{i}{2} K_2\right)^2 \phi - \frac{\hbar^2 b^2 y^2}{2m_1^*} \phi = (W_2 - E)\, \phi \quad . \tag{3.51}$$

If we let $\phi(y) = e^{i/2 K_2 y}\, \eta(y)$, $S' = \left(\frac{m_2}{m_1^*} b^2\right)^{1/4} y$,

and $a' = 2 \frac{(m_1^* m_2)^{1/2}}{m} \left(\frac{W_2 - E}{\hbar \omega_c}\right)$,

then $\eta(y)$ obeys an equation analogous to (3.13),

$$\frac{d^2 \eta}{dS'^2} + (a' + S'^2)\, \eta = 0 \quad , \tag{3.52}$$

for which there are two solutions η_1 and η_2 .

Let us define the turning points y_1', y_2' and y_3' analogously to y_1, y_2 and y_3 (see Figure 2) except shifted to the left by $\frac{1}{2} r_1$, and let $\varkappa(y) = k(y) - \frac{1}{2} K_2$. Then the asymptotic expressions (3.18) and (3.19) can be taken over, for $y > 0$

$$\eta_1 \to \frac{e^{1/2\ a'\ \pi}}{\sqrt{v}} \exp\ (i \int_{y_3'}^{y} \varkappa\ dy) \quad , \tag{3.53}$$

and for $y < 0$,

$$\eta_1 \to \frac{C'}{\sqrt{v}} e^{1/4\ a'\ \pi} \exp\ (-i \int_{y}^{y_2'} \varkappa\ dy) - \frac{i}{\sqrt{v}} \exp\ (i \int_{y}^{y_2'} \varkappa\ dy), \tag{3.54}$$

where $$C' = (\frac{2}{\pi})^{1/2} (\frac{|a'|}{2e})^{-1/2\ ia'} \Gamma(\frac{1}{2} + \frac{1}{2}\ ia') \cosh \frac{1}{2}\ a'\pi \quad .$$

The second solution, η_2, gives the complex conjugate of (3.53) and of (3.54). Multiphying (3.53) and (3.54) by the factor $e^{i/2\ K_2 y}$ gives the form of $\phi(y)$ near the origin.

From (3.50), it is easy to see that the WKB solutions approach

$$\phi(y) = \frac{1}{\sqrt{v}} \exp\ i(\ \frac{1}{2}\ K_2 y \pm i \int^{y} \varkappa\ dy) \quad , \tag{3.55}$$

for y near the origin, and join onto the solutions

$$e^{i/2\ K_2 y}\ \eta_1 \qquad \text{and} \qquad e^{i/2\ K_2 y}\ \eta_2 \quad .$$

Hence, the connection formulas are given by equations like (3.21), (3.22), (3.27), and (3.28) if we replace p and q by p' and q'. The primes denote replacing a by a' in α and in (3.32) and (3.33).

If the open orbit region is sufficiently large, the WKB solutions are accurate for the entire zone except near the origin. The Bloch condition can then be imposed, and the quantization condition can be derived as for electron orbits. The only difference between the hole orbits and the electron orbits is the way in which energy is measured. For electrons,

energy is measured according to $E - W_1$, and for holes, according to $W_2 - E$.

The analysis of this section has been for what could be called one-dimensional coupling because the solutions couple only at points like P_1, P_2 and P_3 in the electron orbits and at P_4 and P_5 in the hole orbits. As a consequence, the energy levels depend only upon a one dimension wavenumber Q.

In a recent paper, Roth (1966) has derived a quantization condition similar to (3.39), but from a different point of view. As a final example of one-dimensional coupling, we examine the self-intersecting orbit (Figure 6) also considered by Roth (1966) and originally studied by Azbel' (1962). In Figure 7, a band structure is shown which would give rise to such orbits. Near the origin, a saddle point exists such as was considered before at $\frac{1}{2} r_1$. The WKB solutions on either side of the origin can be connected with the aid of the p - q formulas. At the turning points y_2 (or y_3) and $-y_2$ (or $-y_3$), we assume complete reflection.

For $y > 0$, the WKB solution is

$$\phi(y) = \frac{B_1}{\sqrt{v}} \exp i\left(\int_{y_1}^{y} k\,dy\right) + \frac{B_2}{\sqrt{v}} \exp -i\left(\int_{y_1}^{y} k\,dy\right), \tag{3.56}$$

and for $y < 0$,

$$\phi(y) = \frac{A_1}{\sqrt{v}} \exp i\left(\int_{y}^{-y_1} k\,dy\right) + \frac{A_2}{\sqrt{v}} \exp -i\left(\int_{y}^{-y_1} k\,dy\right), \tag{3.57}$$

where for $E > W_1$, $y_1 = 0$.

At the origin, we find

$$B_1 = p\,A_2 + q\,B_2 \quad , \quad \text{and} \quad A_1 = q\,A_2 + p\,B_2 \quad . \tag{3.58}$$

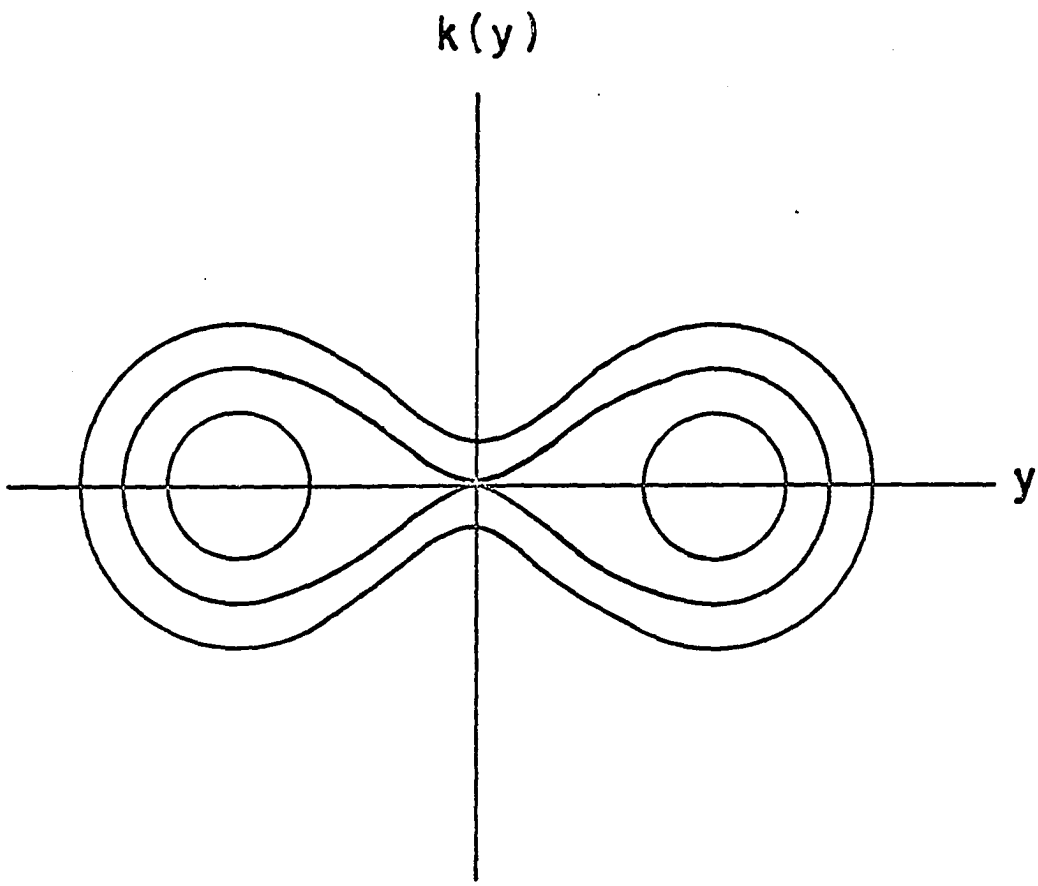


Figure 6. Self-intersecting orbit.

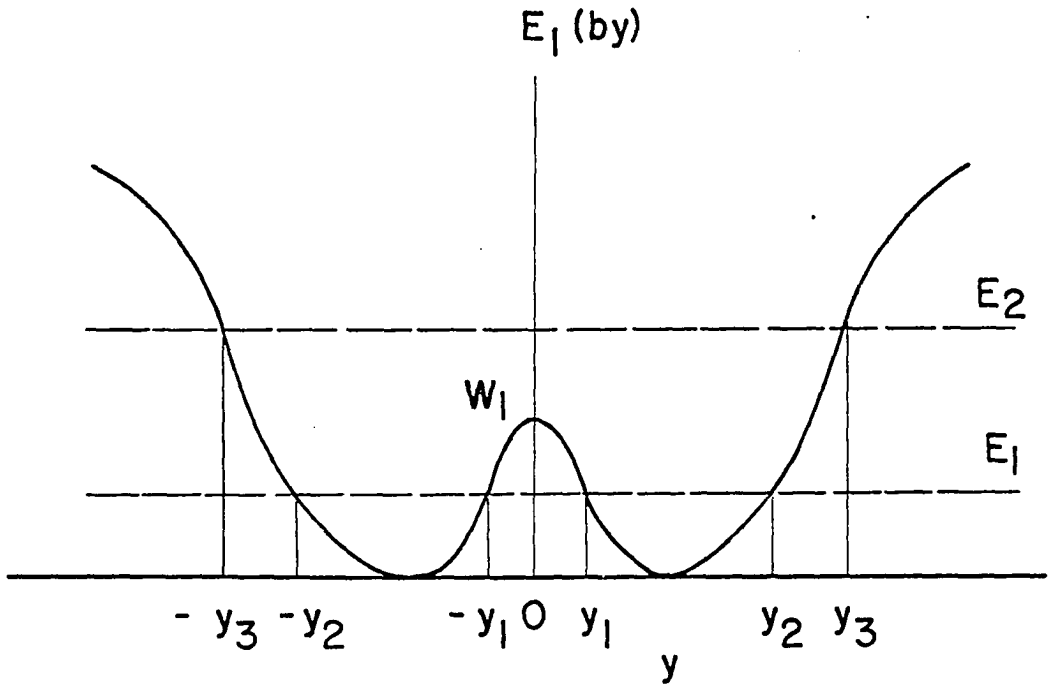


Figure 7. A possible band shape giving rise to a self-intersecting orbit.

At y_2, we have

$$B_2 e^{-i\xi} = -i B_1 e^{i\xi} \quad , \tag{3.59}$$

and at $-y_2$

$$A_2 e^{-i\xi} = -i A_1 e^{i\xi} \quad , \tag{3.60}$$

where $\xi = \int_{y_1}^{y_2} k dy$. Solving the secular determinant, we find the quantization condition

$$\cos (2\xi - \alpha) = - (1 + e^{a\pi})^{-1/2} \quad . \tag{3.61}$$

(3.61) is identical to Azbel's result (1961) when the orbit is symmetric about the origin. The energy levels in the neighborhood of the saddle point are shown in Figure 8. The transition from one quantization scheme to the other is quite rapid, occurring within a few $\hbar\omega_c$ about W_1. The levels are shifted, but remain discrete since there is no infinitely coupled set of orbits involved.

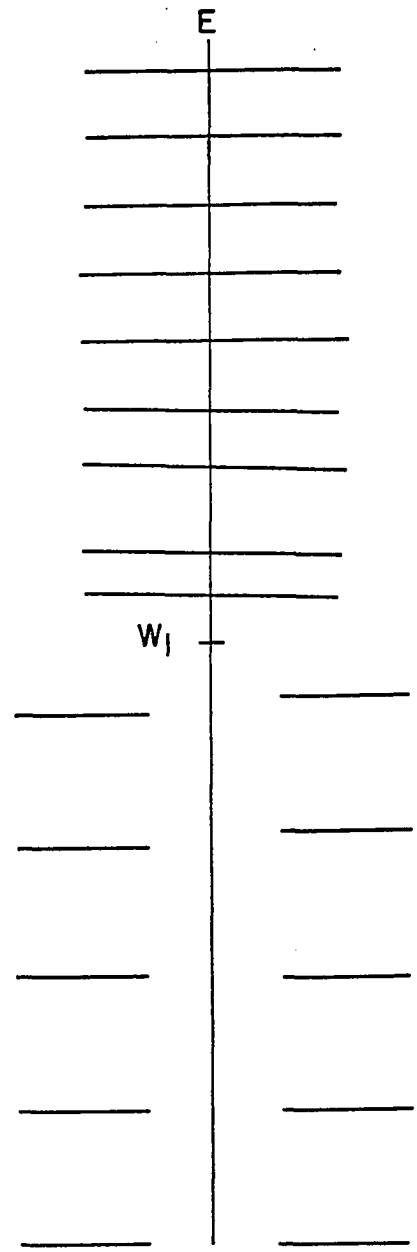


Figure 8. Energy levels near a self-intersecting orbit.

IV. TWO-DIMENSIONAL COUPLING

In the previous section, the energy spectrum was calculated for orbits which were coupled only at

$$y = \pm \frac{1}{2} r_1 \ , \pm \frac{3}{2} r_1 \ . \ . \ . \tag{4.1}$$

or at

$$y = 0, \pm r_1, \pm 2r_1 \ . \ . \ . \tag{4.2}$$

but not both. If now we let W_2 approach W_1 so that only a narrow region of open orbits exists, coupling occurs at both the points (4.1) and (4.2). The intermediate open orbit (T_4 in Figure 3) is an example of such two-dimensional coupling when W_2 is nearly equal to W_1. The term "two-dimensional" arises because $\phi(y)$ can be labeled with a two-dimensional wave-vector (Q_1, Q_2), in place of the one-dimensional Q of Section III.

The WKB solutions are accurate except near the points (4.1) and (4.2), where the solutions are to be connected with the p-q formulas. In Figure 3, it is clear that the pairs of solutions coupled at (4.1) are not the same pairs coupled at (4.2). Hence, we must couple all possible solutions of the type $k(y) + mK_2$ where m is an integer. The WKB solution now becomes an infinite sum over m. We write for $y < y_2'$

$$\phi(y) = \sum_m \frac{A_m}{\sqrt{V}} \exp\, i\left(mK_2 y + \int_y^{y_2'} k\,dy\right)$$

$$+ \sum_m \frac{B_m}{\sqrt{V}} \exp\, i\left(mK_2 y - \int_y^{y_2'} k\,dy\right) \quad , \tag{4.3}$$

and for $y_3' < y$,

$$\phi(y) = \sum_m \frac{C_m}{\sqrt{V}} \exp i\left(mK_2 y + \int_{y_3'}^{y} k\,dy\right) + \sum_m \frac{D_m}{\sqrt{V}} \exp i\left(mk_2 y - \int_{y_3'}^{y} k\,dy\right), \qquad (4.4)$$

where $k(y)$ is the branch depicted by T_4 or the closed orbit branches nearest T_4. That (4.3) and (4.4) are solutions to (3.4) can be verified by direct substitution.

Near $y = 0$, we can see from (3.50) that

$$\int_{y_3'}^{y} k\,dy = \frac{1}{2} K_2 (y - y_3') + \int_{y_3'}^{y} \varkappa\,dy \quad ,$$

and

$$\int_{y}^{y_2'} k\,dy = \frac{1}{2} K_2 (y_2' - y) + \int_{y}^{y_2'} \varkappa\,dy \quad , \qquad (4.5)$$

so for a given m, A_{m+1} and C_m represent outgoing waves while B_m and D_{m+1} represent incoming waves near $y = 0$.

The connection formulas give

$$C_m e^{-i/2\, K_2 y_3'} = p' B_m e^{-i/2\, K_2 y_2'} + q' D_{m+1} e^{i/2\, K_2 y_3'} \quad ,$$

and

$$A_{m+1} e^{i/2\, K_2 y_2'} = q' B_m e^{-i/2\, K_2 y_2'} + p' D_{m+1} e^{i/2\, K_2 y_3'} \quad . \qquad (4.6)$$

The appearance of "m + 1" terms in (4.6) reflects the two-dimensional character of the problem, because the coupling at $y = 0$ is between "m" and "m + 1" solutions while the coupling at $\frac{1}{2} r_1$ involves only "m" solutions. At $\frac{1}{2} r_1$, the connection formulas give after imposing the Bloch condition

$$B_m e^{-i(\xi + Q_1 r_1)} = p\, C_m e^{i\xi} + q\, A_m e^{i(\xi + Q_1 r_1)} ,$$

and

$$D_m e^{-i\xi} = q\, C_m e^{i\xi} + p\, A_m e^{i(\xi + Q_1 r_1)} , \qquad (4.7)$$

where

$$\xi = \int_{y_1}^{y_2'} k\,dy \quad .$$

We can solve (4.6) and (4.7) if we assume that

$$A_{m+1} = e^{iQ_2 r_2} A_m ,$$

and

$$D_{m+1} = e^{iQ_2 r_2} D_m , \qquad (4.8)$$

where $r_2 = \frac{K_2}{b}$ and Q_2 is a wavenumber of range $\frac{2\pi}{r_2}$. The secular equation gives the quantization condition after some manipulations,

$$\cos\left[2\xi + \tfrac{1}{2} K_2 (y_3' - y_2') + \alpha + \alpha'\right] = \frac{\cos Q_1 r_1}{\left[(1+e^{-a\pi})(1+e^{-a'\pi})\right]^{1/2}} + \frac{\cos Q_2 r_2}{\left[(1+e^{a\pi})(1+e^{a'\pi})\right]^{1/2}} \quad . \qquad (4.9)$$

It can be shown that (4.9) gives the correct results for one-dimensional

coupling when W_2 exceeds W_1 by a few $\hbar\omega_c$ or more. It is also clear that for all closed orbits, except those near open orbits, the energy levels are essentially discrete. For $W_2 = W_1$, the relative line width at $E = W_1 = W_2$ ($a = a' = 0$) is unity and significant broadening extends roughly twice as far into the discrete region of the spectrum as in the case of one-dimensional coupling. The dependence of the eigenvalues on a two-dimensional wavevector (Q_1, Q_2) is similar to the magnetic breakdown case in hexagonal metals (Pippard 1964, Chambers 1966).

The two-dimensional coupling case is particularly important because the effective Hamiltonian solution can be related to the actual solution of the Schrödinger equation (1.4) in an interesting manner. In Section II, it was shown that the eigenvalues are independent of k_x, but from group theory (Brown 1964) we know that there must indeed be some dependence upon the x component, as well as the y component, of some wavevector. As we shall demonstrate, the wavevector (Q_1, Q_2) serves this purpose and thus makes the effective Hamiltonian analysis consistent with the requirements of group theory.

In (2.5), a simple relationship between $\Psi(\underline{r})$ and $X(\underline{r})$ was given for the tight binding case in the absence of a magnetic field. When a field exists in any general band structure we take the form to be that given by Brown (1964) as derived from group theory,

$$X(\underline{r}) = \sum_j \Psi(\underline{R}_j)\, u(\underline{r}, \underline{R}_j) \quad , \tag{4.10}$$

where now $u(\underline{r}, \underline{R}_j)$ is the magnetic analog of the Wannier functions.

The general form of $\Psi(\underline{r})$ for our model is from (2.9), (4.3), (4.4),

and (4.8)

$$\Psi(\underline{r}) = e^{ik_z z + ik_x x - i\frac{b}{2}xy} \sum_m e^{i[mK_2(y - \frac{k_x}{b}) + mQ_2 r_2]} g(y - \frac{k_x}{b}) , \quad (4.11)$$

where g(y) is of the form (except near the turning points)

$$g(y) = \frac{A}{\sqrt{V}} \exp\left(i\int^y k\,dy\right) + \frac{B}{\sqrt{V}} \exp\left(-i\int^y k\,dy\right) . \quad (4.12)$$

In (4.10), only the value of $\Psi(\underline{r})$ at $\underline{R}_j$ is important. Since $K_2 Y_j$ equals an integral number of 2π and $br_2 = K_2$, it is easy to see that the infinite sum vanishes unless

$$k_x = Q_2 + \mu\, 2\frac{\pi b}{K_2} , \quad (4.13)$$

where μ is an integer. Although the eigenvalues are formally independent of k_x, the actual wave function vanishes unless (4.13) is satisfied, so in effect the eigenvalues do depend upon k_x. The wavefunction and the eigenvalues also depend upon Q_1 since g(y) is of the form

$$g(y + r_1) = e^{iQ_1 r_1} g(y) . \quad (4.14)$$

Since r_1 and r_2 are much larger than the lattice spacings (typically 10^2 to 10^3 times larger), Q_1 and Q_2 span only a small fraction of the Brillouin zone. One can, in fact, show that the fraction spanned is the same as predicted by group theory. Following Brown (1964), we require b to satisfy

$$b = \frac{2\pi}{Na_1 a_2} , \quad (4.15)$$

where N is an integer, a_1 and a_2 are the lattice spacings and the x and y

directions. A requirement such as (4.15) is necessary if periodic boundary conditions are to be imposed upon a finite volume (Brown 1964).

Since $br_1 = K_1$ and $K_1 = \frac{2\pi}{a_1}$, (4.15) implies that

$$r_1 = Na_2 \quad . \tag{4.16}$$

Similarly, for r_2 we have

$$r_2 = Na_1 \quad . \tag{4.17}$$

The range of Q_1 is $\frac{2\pi}{r_1}$, which is, from (4.16), $\frac{2\pi}{Na_2}$. Likewise, the range of Q_2 is $\frac{2\pi}{Na_1}$. The range of Q_1 and the range of Q_2 coincide with those described by Brown, so the proper fraction of the Brillouin zone is spanned.

One can also show that the effective Hamiltonian formalism accounts for all the states and the appropriate degeneracies in accordance with group theory. In a unit area of the xy plane, there are $\frac{1}{(2\pi)^2}\left(\frac{2\pi}{Na_1}\right)\left(\frac{2\pi}{Na_2}\right)$ states in the fraction of the Brillouin zone spanned by Q_1 and Q_2. Just as in the group theory approach, the states are degenerate with respect to μ in (4.13). If we allow μ to take on N values, the range of k_x is $\frac{2\pi}{a_1}$, and the total number of states per unit area for a given k_z and n (Landau level quantum number) is $\frac{1}{Na_1a_2}$, which agrees with Brown. It would, therefore, appear that the effective Hamiltonian formalism is completely consistent with the dictates of group theory.

Since the eigenvalues and eigenfunctions found in the effective Hamiltonian approach are of the form required from group theoretical considerations of the exact Schrödinger equation (1.4), it would seem that the analysis is correct, and that no source of level broadening due to the

lattice potential has been omitted. Hence, the Landau levels in a perfect crystal are discrete even in the presence of the strong lattice potential of a real metal except when some type of infinite coupling of the orbits exists.

V. OTHER SOURCES OF LEVEL BROADENING

As shown by Pippard (1962, 1964) and by Chambers (1966), magnetic breakdown can cause significant level broadening. The manner in which the levels are broadened is similar to the intraband effects studied above in that degenerate orbits (in different bands) are infinitely coupled to lift the degeneracies. Intraband effects take place at the Fermi level, E_F, only if

$$\frac{\hbar\omega_c}{|E_F - W_1|} > 1 \quad , \tag{5.1}$$

unless the effective masses are extremely small, whereas interband effects (magnetic breakdown) occur when (Ziman 1964, p. 282)

$$\frac{\hbar\omega_c E_F}{E_{gap}^2} > 1 \quad , \tag{5.2}$$

where E_{gap} is the energy gap between bands at the zone boundary. The requirement for intraband effects (5.1) is much more stringent than for magnetic breakdown (5.2) since it is rare that the Fermi energy will approach a saddle point, W_1, by less than typical values of E_{gap}. The factor E_F/E_{gap} is of the order of 10 to 10^3 (or more in some cases of spin orbit splitting).

The analyses of magnetic breakdown by Pippard and by Chambers are more or less semiclassical and appeal largely to one's intuition. The present analysis of intraband effects can be extended to magnetic breakdown in order to provide a partial justification of their analysis within

the framework of the effective Hamiltonian formalism.

In Figure 9, the form of k(y) for Pippard's (1962) network model (a one-dimensional model) for orbits at an energy E is shown. Pippard has assumed only one Fourier coefficient of the lattice potential to be present. The shaded lens orbits are in a higher energy band than the continuous open orbits in this nearly free electron band structure. Magnetic breakdown is said to occur at points such as A and B. In Figure 10a, a close-up of the point A is shown. In the gap region between y_1 and y_2, the wave function is not oscillatory but is exponentially increasing or decreasing since no real values of k(y) for the energy E exist. In other words, the gap region behaves as if a barrier were present.

We can draw some general conclusions without specifying the exact nature of the barrier. The amplitudes of the WKB solutions on either side of the gap must be connected via the p-q formulas (3.21), (3.22), (3.27), and (3.28), where now p and q are not given directly by (3.32) and (3.33), but by some generalization of (3.32) and (3.33). As Pippard (1962) has shown, $|p|^2 + |q|^2 = 1$ and $pq^* + p^*q = 0$. It is clear that (3.32) and (3.33) satisfy these conditions as they must since these conditions surely hold whether the barrier is due to intraband effects or interband effects.

The magnitude of p has been discussed by a number of authors including Harrison (1962), Blount (1962), Pippard (1962), and Chambers (1966). The most common form of $|p|$ is

$$|p| = e^{-H_o/H} , \tag{5.3}$$

where H_o is a critical field which can be realized experimentally in such

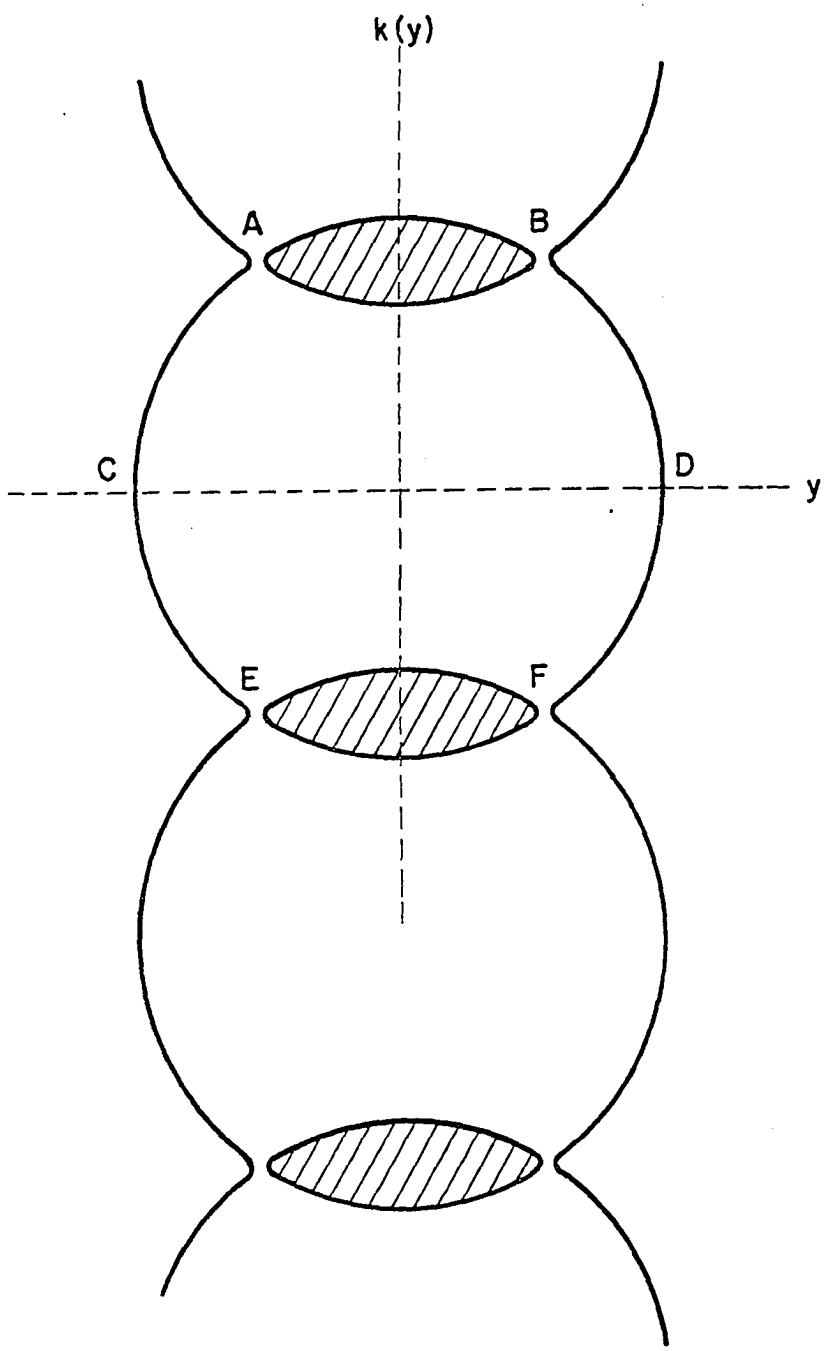


Figure 9. Linear network model for magnetic breakdown (Pippard 1962). Shaded portions represent lens orbits.

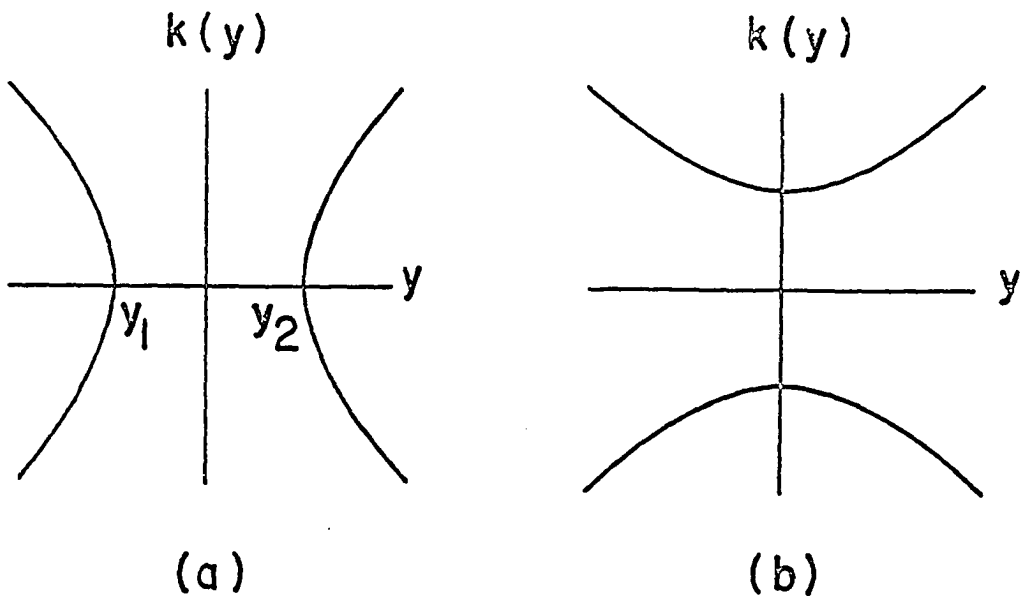


Figure 10. Two choices of the k(y)-y coordinate system which coincide with the principal axes of a saddle point.

metals as Mg (Falicov and Stachowiak 1966).

When H_o is extremely large, no breakdown occurs and $p = 0$. In this limit, we have total reflection at y_1 and y_2 (in Figure 10a), and from the analogous case of total reflection in the intraband case we take $q = -i$. In the limit that H_o/H is nearly zero, the orbits must be essentially free electron orbits and there can be no phase change in the transmitted wave, so that $p = 1$. It seems reasonable, therefore, to regard p as real and q as pure imaginary for all values of H_o/H. Such a choice satisfies $pq^* + p^*q = 0$. (This is just opposite to Pippard (1962) who arbitrarily took p imaginary and q real.) Hence, we have

$$p = e^{-H_o/H} , \tag{5.4}$$

and

$$q = -i\,(1 - p^2)^{1/2} . \tag{5.5}$$

At the points C and D in Figure 9, total reflection occurs since we assume no coupling to other orbits at these points. The WKB wave function for $C < y < A$ is (we denote y_A by A and y_C by C and ignore the finite gap width at A)

$$\phi(y) = \sum_m \frac{A_m}{\sqrt{V}} \exp i\left(mK_2 y + \int_y^A k\,dy\right) + \sum_m \frac{B_m}{\sqrt{V}} \exp i\left(mK_2 y - \int_y^A k\,dy\right) , \tag{5.6}$$

where K_2 is the reciprocal lattice vector in the k_y direction (the separation of the lens orbit centers for example). For $A < y < B$,

$$\phi(y) = \sum_m \frac{C_m}{\sqrt{V}} \exp i\left(mK_2 y + \int_A^y k\,dy\right) + \sum_m \frac{D_m}{\sqrt{V}} \exp i\left(mK_2 y - \int_A^y k\,dy\right) . \tag{5.7}$$

Finally, for $B < y < D$,

$$\phi(y) = \sum_m \frac{E_m}{\sqrt{V}} \exp\, i\left(mK_2 y + \int_B^y k\,dy\right) + \sum_m \frac{F_m}{\sqrt{V}} \exp\, i\left(mK_2 y - \int_B^y k\,dy\right) \quad . \quad (5.8)$$

In (5.6), (5.7), and (5.8), k(y) stands for the branch CABD in Figure 9.

At A, for a given m, the A_{m+1} term represents the outgoing wave for $y < A$ and the B_m term represents the incoming wave for $y < A$. Likewise, C_m stands for the outgoing wave for $y > A$, and D_{m+1} is the incoming wave for $y > A$. Hence, we find

$$A_{m+1} = p\, D_{m+1} + q\, B_m \quad ,$$

and

$$C_m = q\, D_{m+1} + p\, B_m \quad . \quad (5.9)$$

At B, we rewrite (5.7) as

$$\phi(y) = \sum_m \frac{C_m}{\sqrt{V}} \exp\, i\left(mK_2 y - \int_y^B k\,dy + \xi\right) + \sum_m \frac{D_m}{\sqrt{V}} \exp\, i\left(mK_2 y + \int_y^B k\,dy - \xi\right) , \quad (5.10)$$

where $\xi = \int_A^B k\,dy$. Now $D_{m+1}\, e^{-i\xi}$ and, from (5.8), E_m represent outgoing waves, and $C_m e^{i\xi}$ and F_{m+1} represent incoming waves, so

$$D_{m+1}\, e^{-i\xi} = p\, F_{m+1} + q\, C_m\, e^{i\xi} \quad ,$$

and

$$E_m = q\, F_{m+1} + p\, C_m\, e^{i\xi} \quad . \quad (5.11)$$

At C, we can rewrite (5.7) as

$$\phi(y) = \sum_m \frac{A_m}{\sqrt{V}} \exp\, i\left(mK_2 y - \int_c^y k\,dy + \zeta\right) + \sum_m \frac{B_m}{\sqrt{V}} \exp\, i\left(mK_2 y + \int_c^y k\,dy - \zeta\right) , \quad (5.12)$$

where $\zeta = \int_c^A k\,dy$. So $A_m e^{i\zeta}$ is the incoming wave and $B_m e^{-i\zeta}$ is the outgoing

wave, thus

$$B_m e^{-i\zeta} = - i A_m e^{i\zeta} \quad . \tag{5.13}$$

Likewise at D, $E_m e^{i\zeta}$ is the incoming wave and $F_m e^{-i\zeta}$ is the outgoing wave,

$$F_m e^{-i\zeta} = -i E_m e^{i\zeta} \quad . \tag{5.14}$$

Again, we assume that a "m + 1" term equals $e^{iQ_2 r_2}$ times the "m" term.

The set of equations (5.9), (5.11), (5.13) and (5.14) will then have a solution if the secular determinant vanishes. The quantization condition becomes

$$\cos Q_2 r_2 = \frac{q^2 \cos (2\zeta - \xi) - \cos (2\zeta + \xi)}{2|q| \cos \xi} \quad , \tag{5.15}$$

which is the same as Pippard's (1962) result except that we have correctly included the factor of $\pi/2$ when a phase integral is set equal to $(n + \frac{1}{2})\pi$. For example, when $q \to 0$, (5.15) implies that $\cos \xi = 0$ or $\xi = (n + \frac{1}{2})\pi$, where Pippard's analysis would give $\sin \xi = 0$ or $\xi = n\pi$.

In a hexagonal metal, such as Mg, where the breakdown coupling is two-dimensional (Pippard 1964, Chambers 1966), the semiclassical treatment is restricted to field values $H = \hbar/4\pi \, Ne|\underline{a}_1 \times \underline{a}_2|$, where $\underline{a}_1$ and $\underline{a}_2$ are basic vectors of the crystal lattice in the plane normal to $\underline{H}$, and N is an integer of the order of 10^3. Such a requirement arises because one wants the network of classical electron trajectories in real space to repeat itself in an integral number of lattice vectors. This means, for example, that orbit centers always fall at the same point in the unit cell. No

such restrictions are necessary in the effective Hamiltonian formalism of breakdown since we do not concern ourselves directly with the crystal lattice. In essence, the effective Hamiltonian formalism is in reciprocal space and one never needs to refer to the direct space.

Another source of level broadening could be crystal imperfections such as internal strains and dislocations (Pippard 1965, Chambers ca. 1967). Essentially no quantitative experimental information is available, except that the amplitudes of de Haas-van Alphen oscillations seem to depend upon the thermal history of the specimens studies.*

Let us first consider a small, periodic strain. If the period of the strain were to coincide with an integral number of lattice spacings, Na, it might at first appear that such a strain would be serious since it breaks the band structure into N subbands separated by small gaps. (The reciprocal lattice in the direction of the strain is now $\frac{1}{N}\frac{2\pi}{a}$ in place of $\frac{2\pi}{a}$.) However, the gaps separating the subbands are so small that the effect of the broken symmetry is minute.

We can think of the strain introducing an additional potential (Ziman 1964, p. 177-178)

$$\delta V(\underline{r}) = \sum_{ij} E_{ij} W_{ij} e^{i\underline{\tau}\cdot\underline{r}} \quad , \tag{5.16}$$

where E_{ij} is a deformation potential tensor and $W_{ij} e^{i\underline{\tau}\cdot\underline{r}}$ is the strain tensor. The presence of the rest of the Fermi sea screens δV, so that the effective potential is (5.16) reduced by the static dielectric constant,

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* I am indebted to Dr. A. V. Gold and Mr. R. A. Phillips for discussions of this point.

$\epsilon(\underline{\tau})$, (Ziman 1964, p. 129-132)

$$\epsilon(\underline{\tau}) = 1 + \frac{\lambda^2}{\tau^2} \quad , \tag{5.17}$$

where $\frac{1}{\lambda}$ is the screening radius.

For a longitudinal strain, for example, the size of the gaps between the subbands must be of the order of $\frac{E_{11} W_{11}}{\epsilon(\underline{\tau})}$. Typical values of the parameters involved are

$$E_{11} = 10 \text{ eV}$$
$$W_{11} = 10^{-3}$$
$$\lambda = 10^{7} \text{ cm}^{-1}$$
$$\tau = 10^{4} \text{ cm}^{-1} \quad .$$

So $\epsilon(\underline{\tau}) = 10^{6}$, and the gap is of the order of 10^{-8} eV. Typical values of $\hbar\omega_c$ are of the order of 10^{-4} to 10^{-3} eV, so the gap is considerably smaller than $\hbar\omega_c$.

Another, and perhaps more convincing, way of treating the strain is to consider the screened deformation potential as a perturbation. We consider only the discrete levels since the open orbits are already continuous and the additional broadening would be of no consequence. In the effective Hamiltonian formalism, let us assume that the strain is along the y direction. The perturbation will remove the degeneracy among the various solutions localized in different valleys or zones. An upper bound to the matrix elements between different solutions is the maximum value of the potential which is, as shown above, 10^{-8} eV and is much less than $\hbar\omega_c$. Hence, it does not appear that internal strains give rise to any significant broadening.

The effect of dislocation planes can be important, however, as will be demonstrated below in a simple example. Consider the effect of a dislocation plane perpendicular to the y axis falling somewhere between the turning points y_1 and y_2 in Figure 2. The WKB solutions are not accurate at the dislocation plane since it must surely act as a barrier of some type. The solutions on either side of the barrier can be connected with a generalization of the p-q formulas as in the case of magnetic breakdown. Let us again take p to be real and $q = -i(1-p^2)^{1/2}$. Let $y = d$ be the point where the dislocation plane falls.

One can show quite simply that the quantization condition for discrete levels is (the analysis is similar to that of the self-intersecting orbit in Section III)

$$\cos(\xi_1 + \xi_2) + |q| \cos(\xi_2 - \xi_1) = 0 \quad , \tag{5.18}$$

where $\xi_1 = \int_{y_1}^{d} k\,dy$ and $\xi_2 = \int_{d}^{y_2} k\,dy$.

Since the dislocation plane can fall at any point d, between y_1 and y_2 or their equivalents in another valley, $\cos(\xi_2 - \xi_1)$ can be any value between -1 and 1. Normally $|q|$ will be small or else the Landau levels will be completely destroyed. So letting $\xi_1 + \xi_2 = (n + \frac{1}{2})\pi + \Delta\pi$, we find for small $|q|$

$$\Delta\pi = (-1)^n |q| \cos(\xi_2 - \xi_1) \tag{5.19}$$

The relative level width is then

$$\delta n = \frac{2}{\pi} |q| \tag{5.20}$$

If $|q| = 0.1$, the broadening would certainly be detectable experimentally in the de Haas-van Alphen effect.

VI. DISCUSSION

A detailed analysis of a simplified model of the effective Hamiltonian formalism has been given. The simplifications assumed were made primarily for convenience and clarity, and were not essential to the analysis. The conclusions drawn from the model are, in fact, correct beyond its range of validity. As a bridge between the model and the general problem, a brief description of the analysis of the general problem will be indicated.

In the general problem, where the energy band function $E(\underline{k})$ can not be separated as in (3.1), Zil'berman (1957b) and Blount (1962) have shown that a WKB solution exists where now k(y) is given by

$$E(-by, k(y), k_z) = E \quad , \tag{6.1}$$

and the velocity is given by

$$V = \frac{1}{\hbar} \left| \frac{\partial E}{\partial k_y} \right| \quad . \tag{6.2}$$

As before, k_z, which is along $\underline{H}$, is a good quantum number.

Blount (1962) has discussed the types of solutions to be expected when $\underline{H}$ (and k_z) are oriented at an arbitrary direction with respect to a symmetry axis. The repetitious pattern of the curves of constant energy for fixed k_z (such as Figure 3) can be quite tortuous, but we should not expect the degeneracies among solutions in different zones to be lifted in the absence of any coupling.

As we have shown in Section II, the general problem can be reduced to an equation in a single variable y. But, this one-dimensional approach is not useful for complicated orbits such as a star-shaped orbit. The

one-dimensional approach only works nicely if the coupling points are of the type of Figure 10a or 10b. That is, when k(y) and y coincide with the principal axes of the saddle point. In the star-shaped orbit, for example, the k(y)-y coordinate system can not be chosen so that all of the coupling points (assumed to be at the tips of the star) are of the two types in Figure 10. The local equations near the coupling point mix k(y) and y since there are cross terms in an expansion of $E(\underline{k})$ about the saddle point. The cross terms complicate the differential equations for $\phi(y)$ when k(y) is replaced by $-i\frac{d}{dy}$.

Perhaps an even simpler approach to the general problem, than that of the model, is an equivalent semiclassical treatment such as Pippard's (1962, 1964) analysis of magnetic breakdown. In the semiclassical approach, we suppose that the electron is a wave packet traveling about a trajectory in real space similar to the k(y)-y curves of Figure 3. The phase change of the wave packet between two points is related to simple geometrical properties of the trajectory as in the Onsager rules. When a wave packet of unit amplitude encounters a coupling point, the amplitude of the transmitted portion is p and the amplitude of the reflected portion is q. Since we have verified the semiclassical approach for a one-dimensional network in Section V, we expect it to be quite useful for the complicated networks found in real metals, if we are not concerned with details such as $\frac{\pi}{2}$ in factors of $(n + \frac{1}{2})\pi$.

Whether we treat the orbits in terms of wave functions or in terms of semiclassical wave packets, the conclusions must be the same as in the model. Significant broadening of the energy levels associated with closed

orbits in a perfect crystal can only occur when there is either intraband coupling, or interband coupling, to other degenerate orbits. Broadening can also arise when dislocation planes are present, but it appears that small periodic strains are effectively screened out, and thus do not give a contribution to the natural line width of the energy levels. Since we have been able to show that the effective Hamiltonian formalism is completely consistent with the requirements of a group theoretical treatment of the exact Hamiltonian, it would appear that no source of level broadening has been omitted, and the analysis given in this investigation is essentially correct.

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